

# Shiba impurity bound states as a probe of topological superconductivity and Fermion parity changing quantum phase transitions

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Spin-orbit coupled superconductors are potentially interesting candidates for realizing topological and potentially non-Abelian states with Majorana Fermions. We argue that time-reversal broken spin-orbit coupled superconductors generically can be characterized as having sub-gap states that are bound to localized non-magnetic impurities. Such bound states, which are referred to as Shiba states, can be detected as sharp resonances in the tunneling spectrum of the spin-orbit coupled superconductors. The Shiba state resonance can be tuned using a gate-voltage or a magnetic field from being at the edge of the gap at zero magnetic fields to crossing zero energy when the Zeeman splitting is tuned into the topological superconducting regime. The zero-crossing signifies a Fermion parity changing first order quantum phase transition, which is characterized by a Pfaffian topological invariant. These zero-crossings of the impurity level can be used to locally characterize the topological superconducting state from tunneling experiments.

**Introduction:** Majorana Fermions (MF) have been the subject of intense recent study, both due to their fundamental interest as a new type of particle with non-Abelian statistics and their potential application in topological quantum computation (TQC)[1–5]. Topological superconductors [6] are promising candidates for the practical solid state realization of MFs [7–14]. A simple topological superconducting (TS) system supporting MFs, which has attracted considerable experimental attention [2], consists of a spin-orbit coupled semiconductor in a magnetic field placed in contact with an ordinary superconductor [10–14]. It has been shown that the semiconductor proposal in one-dimension, i.e. a semiconducting nanowire, can be driven into a TS phase through the appropriate tuning of the semiconductor chemical potential or equivalently, the carrier density [13, 14]. Such nanowires provide a realization of MFs at its ends in the same class as  $p$ -wave superconductors [15, 16]. The TS state is predicted to be realized in the nanowire when ever the chemical potential  $\mu$  with respect to the bottom of one of the electron sub-bands of the nanowire satisfies the constraint  $|\mu| < \sqrt{\Delta^2 + V_Z^2}$ , where  $V_Z$  is the magnetic-field induced Zeeman potential in the wire and  $\Delta$  is the superconducting pairing potential induced in the wire from contact with the  $s$ -wave superconductor [17]. The  $s$ -wave proximity effect on an InAs quantum wire, which also has a sizable SO coupling, may have already been realized in experiments [18]. Therefore, the TS phase in a semiconductor quantum wire may be one of the most experimentally promising approaches to realizing MFs with non-Abelian statistics. In fact, recent experimental results [19] on the semiconducting wire system suggesting the existence of MFs in this system has created a great deal of interest in the physics community [20].

While several schemes such as tunneling and the fractional Josephson effect have been proposed to detect the presence of MFs [10, 13, 14, 16, 21], local probes that

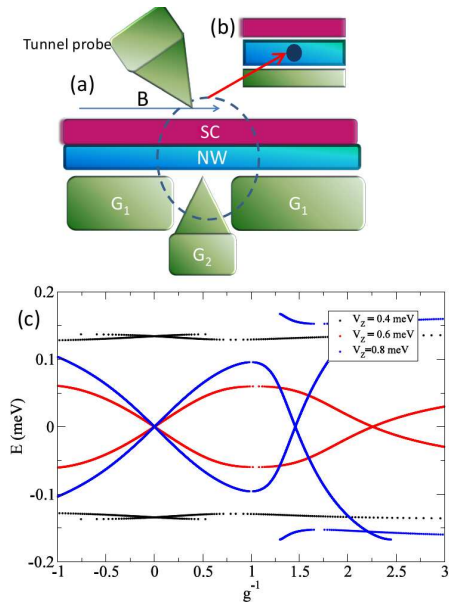


FIG. 1: (Color) (a) Shiba states in a nanowire (NW), which is in a magnetic field  $B$  and in proximity to a superconductor (SC) can be detected as a conductance peak from an STM tip or other tunnel probe near a gate-induced tunable potential  $G_2$ . (b) The gate potential produced by  $G_2$  can be replaced by a local impurity. (c) Shiba bound state energies as a function of inverse impurity strength or impurity transparency  $g^{-1}$  for various values of the Zeeman splitting  $V_Z$  for a topological superconducting nanowire (i.e.  $V_Z = 0.6$  meV (red curve),  $V_Z = 0.8$  meV (blue curve)) shows a characteristic zero-energy crossings, while the wire in the non-topological superconducting phase (i.e.  $V_Z = 0.2$  meV (black curve)) shows weakly bound Shiba states.

characterize the TS state of the wire are still missing. The need for such local characterization becomes specifically urgent because of the presence of disorder in realistic semiconducting wires. The absence of time-reversal symmetry leaves the proximity-induced superconducting

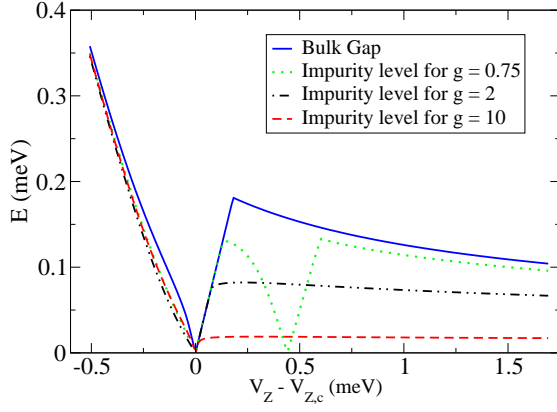


FIG. 2: (Color online) Impurity bound state energy and bulk gap as a function of Zeeman splitting for various values of impurity strength  $g$ . The values of  $V_Z$  greater than the critical value  $V_Z \sim 0.7$  meV, at which the bulk gap vanishes, support a topological superconducting phase in the nanowire. The Shiba bound state energies are seen to be deeply bound with energies significantly below the bulk gap only in the topological superconducting phase. Such Shiba bound states might contribute to near-zero bias conductance that is robust over a range of Zeeman potentials seen in recent experiments [19]. Here we have chosen  $\mu = 0.2$  meV,  $\Delta = 0.5$  meV and the spin-orbit coupling  $\alpha = 0.3$  corresponding to a spin-orbit energy  $E_{SO} \approx 50 \mu\text{eV}$  [36].

gap of the nanowire susceptible to disorder [23–27], which is predicted to lead to subgap states in the bulk of the wire [22, 23]. Such disorder induced gapless states can broaden the MFs into Majorana resonances and eliminate the fractional Josephson effect [28, 29]. Therefore, while probes of topological superconductivity such as the fractional Josephson effect, provide a true characterization of the topological degeneracy associated with MFs, they cannot distinguish if some part of the disordered wire is locally in an essentially TS phase. Scanning tunneling microscopy (STM) of superconductors has provided one such route to experimentally characterizing, in a local way, the superconducting state of superconductors such as the high-Tc cuprate superconductors [30]. In fact, the STM spectrum of impurities allows the characterization of not only the superconductor [31], but also the effect of different impurities on the superconducting state [32]. Magnetic impurities in spin-singlet superconductors lead to Shiba states, which appear as sharp features in tunneling spectra [33]. Tuning the strength of the impurity has been predicted, in principle, to lead to a local quantum phase transition (QPT) [34, 35]. Therefore, it is natural to expect that studying the tunneling spectra around impurities in wires might allow one to understand the TS character of each part of the wire in a local way.

In this paper, we show that the three ingredients of spin-orbit coupling, Zeeman splitting and  $s$ -wave superconductivity required to realize the TS phase in nanowires are also the ingredients that realize sub-gap

Shiba states bound to non-magnetic impurities. Such Shiba states in semiconductor nanowires in proximity to a superconductor can be probed by a STM or tunnel probe arrangement shown in Fig. 1(a,b). For static impurities, we find that the energy associated with the Shiba-state can be tuned to cross zero as seen in Fig. 1(c), providing a realization of the previously predicted Fermion-parity changing transition [35] in a scenario where it might be easier to tune the impurity strength. Such a zero-crossing will be shown to be associated with a local version of the Pfaffian topological invariant that may be used to characterize the TS phase. By a numerical study of models for the semiconducting nanowires, we find (see Fig. 2) that such strongly bound Shiba states only occur in the TS phase of the nanowires. The energy of these sub-gap states in the TS phase are found to be independent of the Zeeman energy and provide a possible alternative explanation to the recently observed zero-bias conduction peaks [20]. Such sub-gap states may be viewed as a way to destroy the TS gap, which is complementary to the Born approximation approach applicable to short-scale disorder such as surface roughness of the nanowire.

#### Local impurity bound states in superconductors:

To understand the spectrum associated with impurities, we consider the Green function  $G_{\tau\sigma;\tau'\sigma'}(\mathbf{r};\mathbf{r}';E)$  of the superconducting nanowire in the Nambu spinor notation. Here  $\mathbf{r}, \mathbf{r}'$  represent spatial coordinates on the nanowire,  $\sigma, \sigma'$  refer to the spin indices of the electron and  $\tau, \tau' = 0, 1$  represent the particle-hole index, which is needed to describe both the normal and anomalous parts of the Green function of the superconducting nanowire. The Green function  $G$  matrix for an impurity in a superconductor can be calculated using the Dyson equation

$$G(\mathbf{r}\mathbf{r}';E) = G_0(\mathbf{r}\mathbf{r}';E) + \int d\mathbf{r}_1 G^{(0)}(\mathbf{r}\mathbf{r}_1;E)V(\mathbf{r}_1)\tau_z G(\mathbf{r}_1\mathbf{r}';E) \quad (1)$$

where  $V(\mathbf{r}) \propto g\delta(\mathbf{r})$  is the localized impurity potential and  $G_{\tau\sigma;\tau'\sigma'}^{(0)}(\mathbf{r};\mathbf{r}';E)$  is the Green function of a clean superconducting nanowire with a Bogoliubov de-Gennes (BdG) Hamiltonian

$$H_0 = (-\partial_x^2 - \mu + i\alpha\sigma_y\partial_x)\tau_z + V_Z\sigma_z + \Delta\tau_x. \quad (2)$$

In the case of a single-channel wire,  $\mu$  represents the chemical potential,  $\alpha$  is the strength of Rashba spin-orbit coupling,  $V_Z$  the magnetic field induced Zeeman potential and  $\Delta$  represents the proximity induced superconducting pairing potential [10, 13]. The impurity strength  $g$  is inversely related to the transparency  $Z$  of the impurity potential. The matrices  $\sigma_z$ ,  $\tau_x$ , and  $\tau_z$  are Pauli matrices associated with the indices  $\sigma$  and  $\tau$  respectively. The BdG Hamiltonian  $H_0$  can also be used to represent multi-band wires [22, 37, 38] if  $\mu$ ,  $V_Z$ ,  $\Delta$  and  $g$  are taken to be matrices indexed by the channel index. For local

impurity potentials, the energy levels of bound states are determined from the  $\mathbf{r} = \mathbf{r}' = 0$  part of the Dyson equation Eq. 1, which is written as

$$G(00; E) = (1 - gG^{(0)}(00; E)\tau_z)^{-1}G^{(0)}(00; E). \quad (3)$$

The Shiba bound state appears as a pole in the Green function  $G$ , which corresponds to a zero of the matrix

$$\text{Det}[g^{-1} - G^{(0)}(00; E)\tau_z] = 0. \quad (4)$$

Consistent with Anderson's theorem [24, 38], the above equation describing sub-gap states bound to non-magnetic impurities, is found to have no solutions in the absence of a Zeeman potential i.e. for  $V_Z = 0$ . The absence of Shiba states continues to hold, even in the presence of a spatially uniform Zeeman potential  $V_Z \neq 0$ , if the spin-orbit coupling  $\alpha$  vanishes, since the Zeeman splitting does not affect the wave-functions of the BdG Hamiltonian. Therefore, non-magnetic impurities can lead to localized Shiba bound states in wires only in the presence of a combination of Zeeman splitting and spin-orbit coupling, which are precisely the conditions to realize a TS phase.

In contrast, for finite spin-orbit coupling  $\alpha$ , Zeeman potential  $V_Z$  and superconducting pairing potential  $\Delta$ , numerical solutions of Eq. 4 plotted in Fig. 1 show sub-gap Shiba states bound to even non-magnetic impurities. While bound Shiba states are found to exist in the entire range of Zeeman potential  $V_Z > 0$ , one observes that the Shiba states occur deep inside the bulk gap of the nanowire, which is also plotted in Fig. 2, only on the TS phase of the nanowire, i.e.  $V_Z > V_{Z,c} = 0.5$  meV. The TS state of the nanowire can be seen identified in Fig. 2 by the vanishing of the bulk gap in the wire at  $V_Z = V_{Z,c}$ . Thus, the existence of deeply bound Shiba states may be considered as suggestive of the nanowire being in the TS phase.

**Shiba states in the TS phase:** While the detection of a deeply bound Shiba state might suggest the nanowire being in a TS phase, it cannot be taken as a confirmatory test. Here we show that the evolution of the Shiba bound state energy as a function of the strength of the impurity  $g$  (or magnetic field or density; see discussion below) may be used as a precise characterization of the TS phase. This is seen from the numerical results for the Shiba bound state energy in the TS and NTS phases of the nanowire, which are plotted in Fig. 1. The Shiba bound state energy in the TS phase in Fig. 1 shows a characteristic pair of crossings of  $E = 0$  at both zero and non-zero values of the impurity transparency  $g^{-1}$ .

**Parity-changing QPT:** The crossing of the Shiba bound state at  $E = 0$  at vanishing transparency  $g^{-1} \sim 0$  is characteristic of the TS phase. This follows from the fact that an impurity with vanishing transparency  $g^{-1} = 0$  splits the nanowire into two nanowires with a pair of zero-energy MFs at the impurity. The pair of zero-energy

MF split linearly by tunneling across the as the impurity is tuned away from vanishing transparency. The zero-crossing of the energy of a Shiba-state is accompanied by a change of the Fermion-parity of the ground state. This is because the positive and negative energy eigenvalues,  $\epsilon_1(g^{-1}) > 0$  and  $-\epsilon_1(g^{-1}) < 0$  of the BdG Hamiltonian refer to the different occupancies of the associated Fermionic state 1. The ground state of the system at  $g_1^{-1}$  corresponds to the positive energy eigenvalue being unoccupied. When the impurity strength  $g^{-1}$  is tuned from  $g_1^{-1}$  to  $g_2^{-1}$ , so that the positive and negative energy states cross zero and are interchanged i.e.  $\epsilon_1(g_2^{-1}) < 0$  and  $-\epsilon_1(g_2^{-1}) > 0$ , the system reaches a state where the positive energy state 1 is occupied. Such a state with a positive energy eigenvalue occupied is an excited state of the Hamiltonian with  $g_2^{-1}$ . However, this excited state has the same Fermion parity as the ground state at  $g_1^{-1}$ , i.e. before the energy crossing. Since the excited state obtained by tuning the impurity to  $g_2^{-1}$  is related to the ground state at  $g_2^{-1}$  by adding a Fermion, the ground state at  $g_2^{-1}$  must have a different Fermion parity from the ground state at  $g_1^{-1}$ . Therefore, the zero-energy crossing of the Shiba state is associated with a QPT where the ground state of the system changes its Fermion parity. This is analogous to the QPT proposed for tunable magnetic impurities in conventional superconductors [35]. The spin-orbit coupled nanowire provides a realization of this interesting transition using a non-magnetic impurity, which can be tuned by a local gate voltage.

The Fermion parity change associated with zero-energy crossings of Shiba states at vanishing impurity transparency  $g^{-1} \sim 0$  in the TS phase requires the existence of an odd number of zero-energy crossings at finite impurity transparency  $g^{-1} \neq 0$ . This follows from the fact that the total number of zero-energy crossings going from  $g^{-1} = -\infty$  to  $g^{-1} = \infty$  must be even, since both these points are associated with the ground state Hamiltonian of the nanowire with no impurity i.e. at  $g \sim 0$ . Thus, the TS phase is characterized by the Shiba bound state energy crossing zero an odd number of times as the limit of infinite impurity strength  $g \rightarrow \infty$  is approached from at least one of the sides of either strong repulsive impurities or strong attractive impurities.

**Local Pfaffian topological invariants associated with impurities:** To strengthen the argument that the zero-energy crossing is a topological QPT, we compute the fermion parity using the Pfaffian topological invariant [16], which can be written in terms of the BdG Hamiltonian [39]. The Pfaffian topological invariant for a particle-hole symmetric BdG Hamiltonian  $H_{BdG}$  can be written in terms of the particle-hole matrix  $\Lambda = \sigma_y \tau_y$  as  $Q(H_{BdG}) = \text{sgn}(Pf[H_{BdG}\Lambda])$ . The particle-hole matrix  $\Lambda$  is defined so that the particle-hole symmetry of  $H_{BdG}$  can be written as  $H_{BdG}\Lambda = -\Lambda H_{BdG}^*$ , which is equivalent to the condition that  $H_{BdG}\Lambda$  is anti-

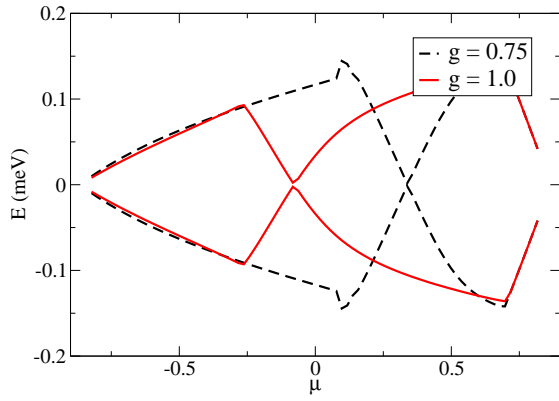


FIG. 3: (Color online) The evolution of the Shiba bound state energy with the local chemical potential show an odd number of crossings in the topological superconducting phase of the nanowire. The chemical potential in the neighborhood of an impurity in a nanowire can be varied, in principle, by a local gate voltage. The zero-energy crossings occur at different values of the local chemical potential for different values of the impurity transparency  $g^{-1}$ .

symmetric, which in turn allows the definition of the Pfaffian  $Pf[H_{BdG}\Lambda]$ . Defining the QPT of the impurity problem requires a local definition of the Pfaffian invariant. To obtain such a local definition we note that zero-energy crossings at an impurity also imply zero-energy crossings of the Green function  $U = G^{(0)}(0, 0; E = 0) - g^{-1}\tau_z$  (see Eq. 4). Since we are considering an impurity in a gapped superconductor  $G^{(0)}$  and the relevant matrix for determining zero-modes  $U = G^{(0)}(0, 0; E = 0) - g^{-1}\tau_z$  is both Hermitean and particle-hole symmetric. Therefore the local Pfaffian invariant is defined as

$$Q(g^{-1}) = \text{sgn} \left( Pf[(G^{(0)}(0, 0; E = 0) - g^{-1}\tau_z)\Lambda] \right). \quad (5)$$

The above Pfaffian invariant can only change sign when the determinant of  $U = G^{(0)}(0, 0; E = 0) - g^{-1}\tau_z$  vanishes, which corresponds to a solution of Eq. 4 at  $E = 0$  and therefore a zero-crossing of Shiba bound state energies. The Fermion parity changing transition of the ground state as a function of impurity strength  $g$  is characterized by the topological invariant  $Q(g^{-1})$  changing sign. Therefore, the local Fermion parity at the impurity can be calculated directly from computing the local Fermion-parity  $Q(g^{-1})$  without computing the Shiba bound states.

Even though the strength of an electrostatically induced impurity in a wire can in principle be controlled by a gate voltage in a simpler way than the tunable magnetic impurity required for  $s$ -wave superconductors [35], tunable non-magnetic impurities also might be difficult to obtain. An alternative approach to locally characterizing a TS phase is to study the evolution of the Shiba bound state energy as one tunes the chemical potential or the magnetic field towards the gap-closing topological

phase transition. It is reasonable to expect a sufficiently strong impurity behaves has an asymptotically stronger effect as one approaches the phase transition. The evolution of the Shiba states across the phase transition for different local impurity strengths, which are plotted in Fig. 2(dotted green) and 3, shows that this is indeed the case. Therefore, the TS phase of the nanowire can also be characterized by the presence of an odd number of zero-energy crossings of the Shiba bound state energy as the applied chemical potential is locally tuned across a QPT.

**Conclusion:** Spin-orbit coupled coupled nanowires together with Zeeman splitting and  $s$ -wave superconductivity, which can be used to realize one-dimensional TS nanowires, are also precisely the ingredients needed to realize sub-gap Shiba states bound to non-magnetic impurities. Similar to magnetic impurities  $s$ -wave superconductors [31], Shiba bound states can also be used to characterize the TS phase of the nanowire. Specifically, only the TS phase of the nanowire is found to support deeply bound Shiba states, whose energies are only weakly Zeeman field dependent. Such low-energy Shiba states found only in the TS phase provides a possible alternative explanation to the recent observations of zero-bias conductance peak, which was interpreted as a signature for the existence of MFs [19]. In the TS phase of the nanowire that the Shiba bound state energy is found to cross zero-energy an odd number of times as one tunes the strength of the impurity. Such zero-crossings of the Shiba bound state energy, besides providing a local characterization of the TS phase of the nanowire, are also intrinsically interesting since they are associated with a Fermion parity changing QPT of the nanowire ground state [35]. For systems where the impurity strength is difficult to tune, we find that similar zero-energy crossings of the Shiba bound state energies for impurities in nanowires in the TS phase can also be obtained by gate tuning the chemical potential. Therefore, the TS phase of spin-orbit coupled semiconducting nanowires can be locally characterized by studying the evolution of Shiba bound state energies, which appear as sub-gap resonances in the tunneling spectrum into the wire. Since most of our results follow from the scattering equation (Eq. 4) from a local impurity, we expect our conclusions to apply to multi-channel nanowires as well as impurities in two-dimensional TS systems. Such local characterizations of the TS phase of the nanowire are particularly useful, since only parts of wires can be expected to enter the TS phase in disordered semiconducting wire.

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